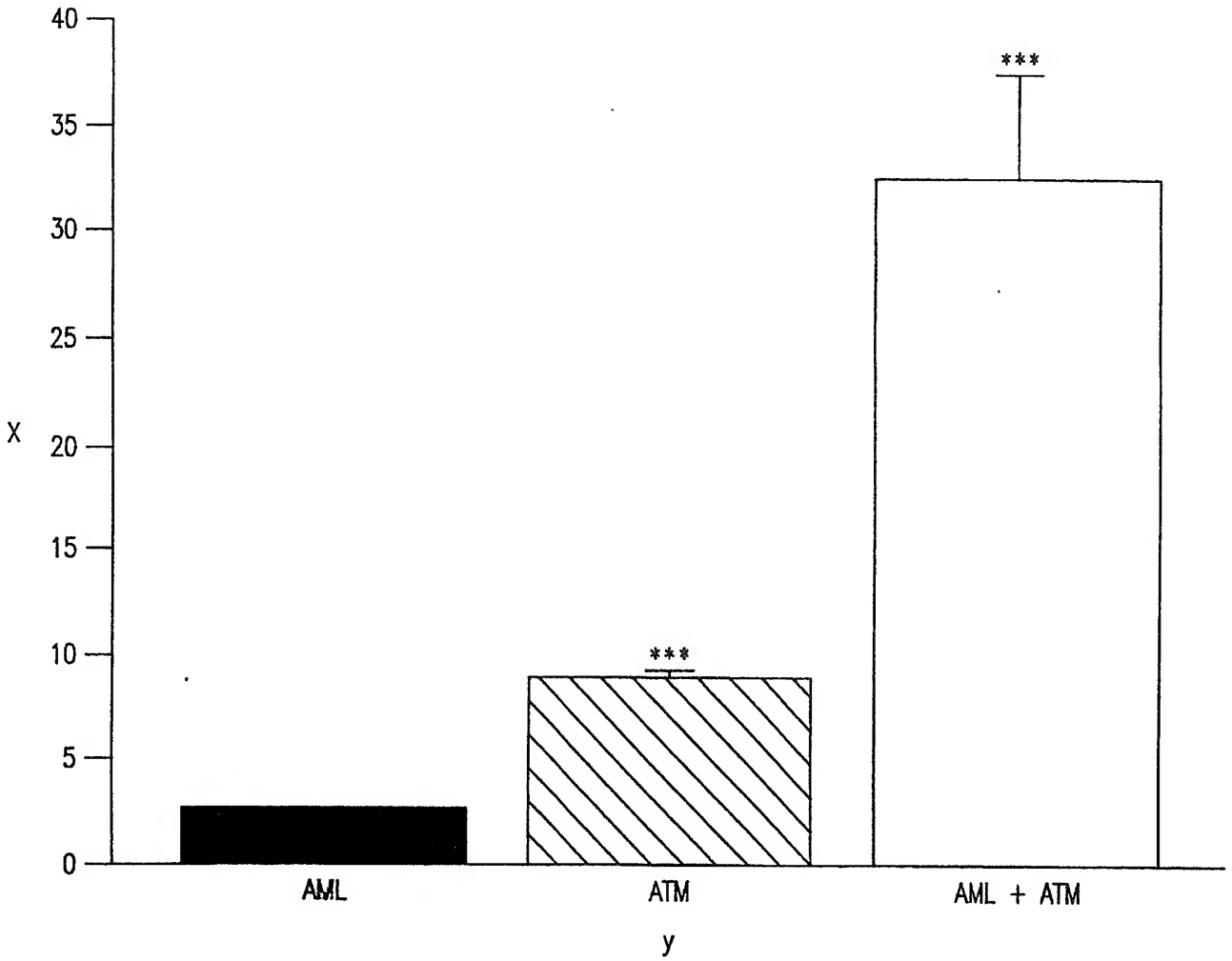

FIG. 1

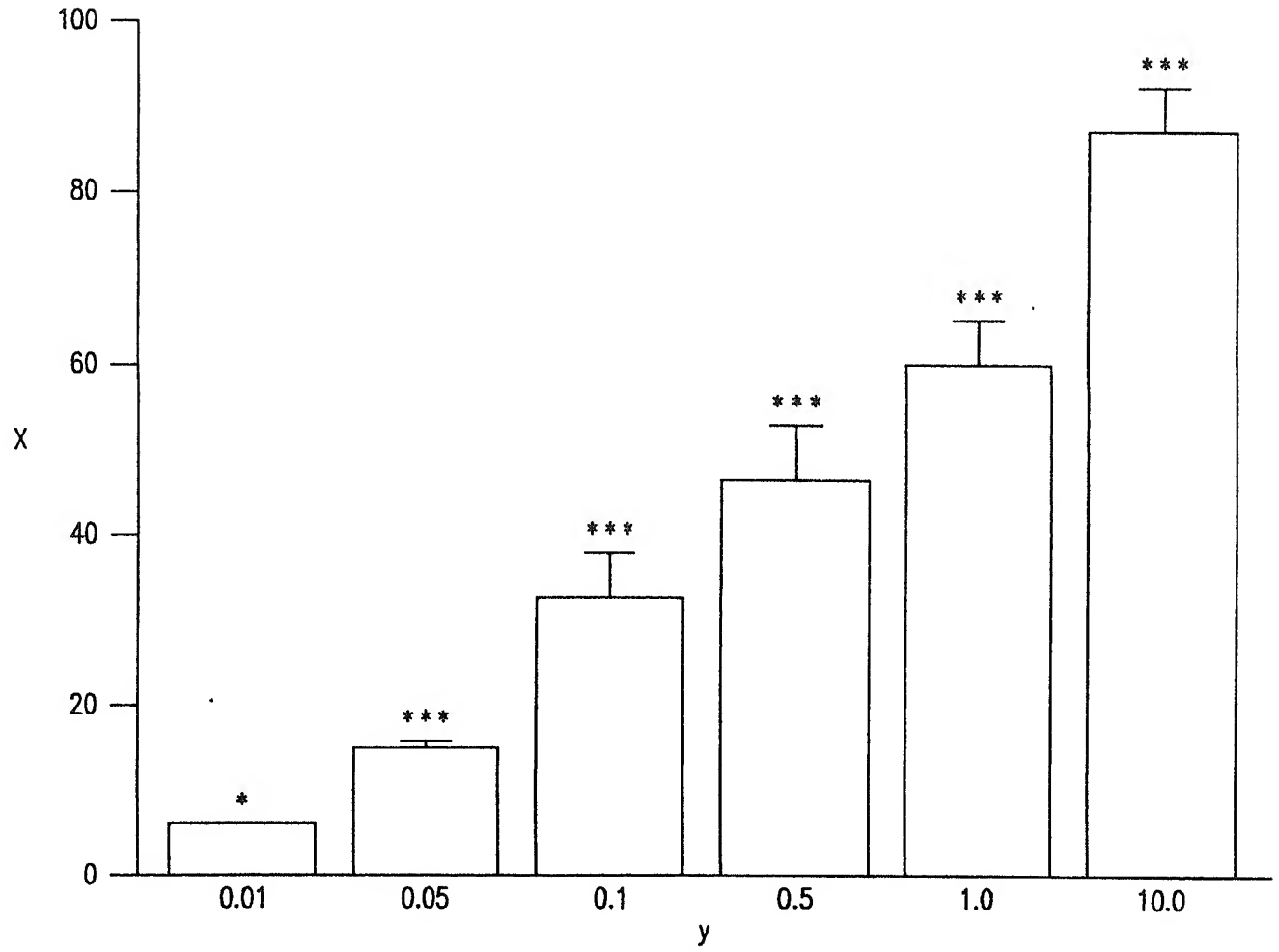

FIG. 2

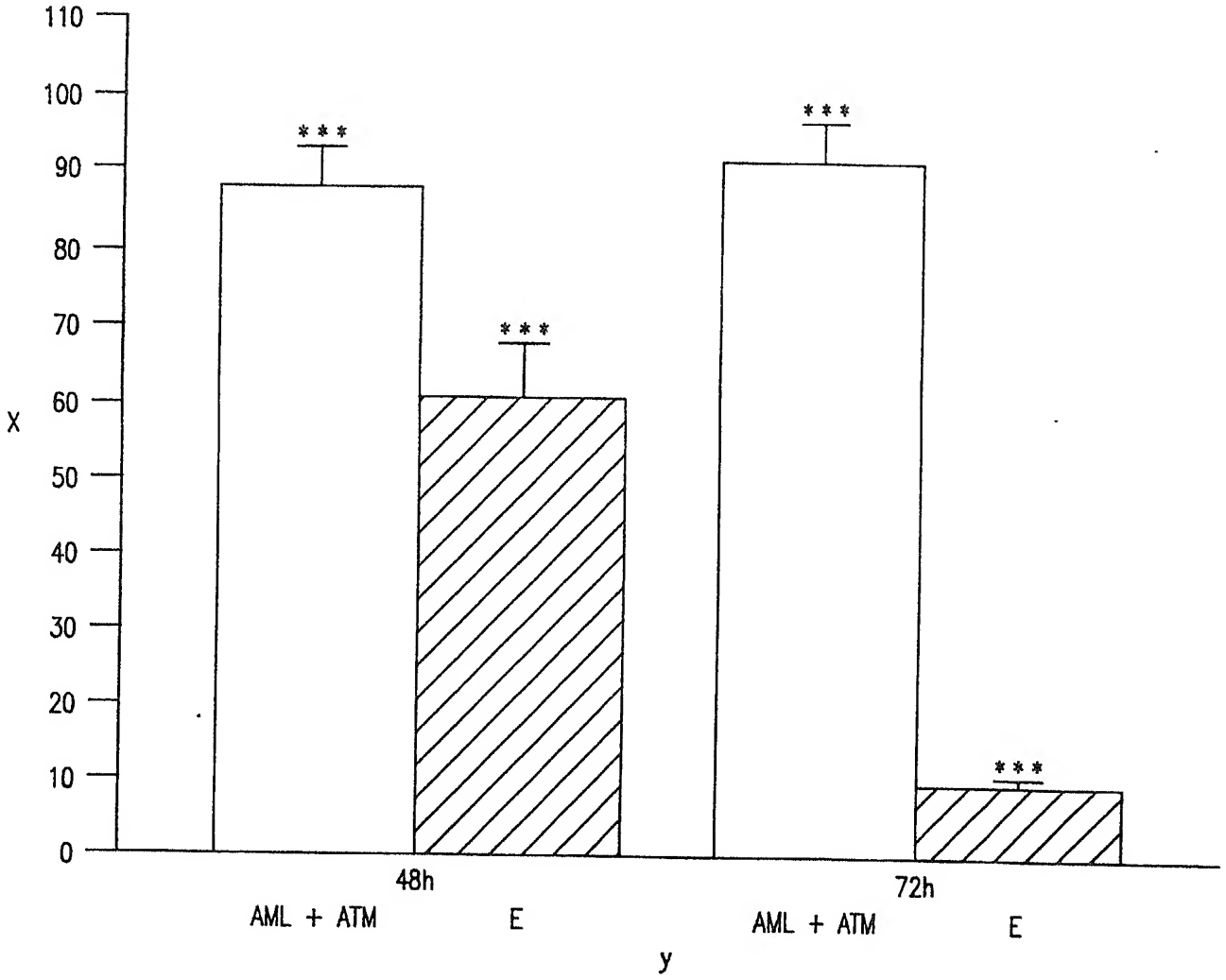

FIG. 3

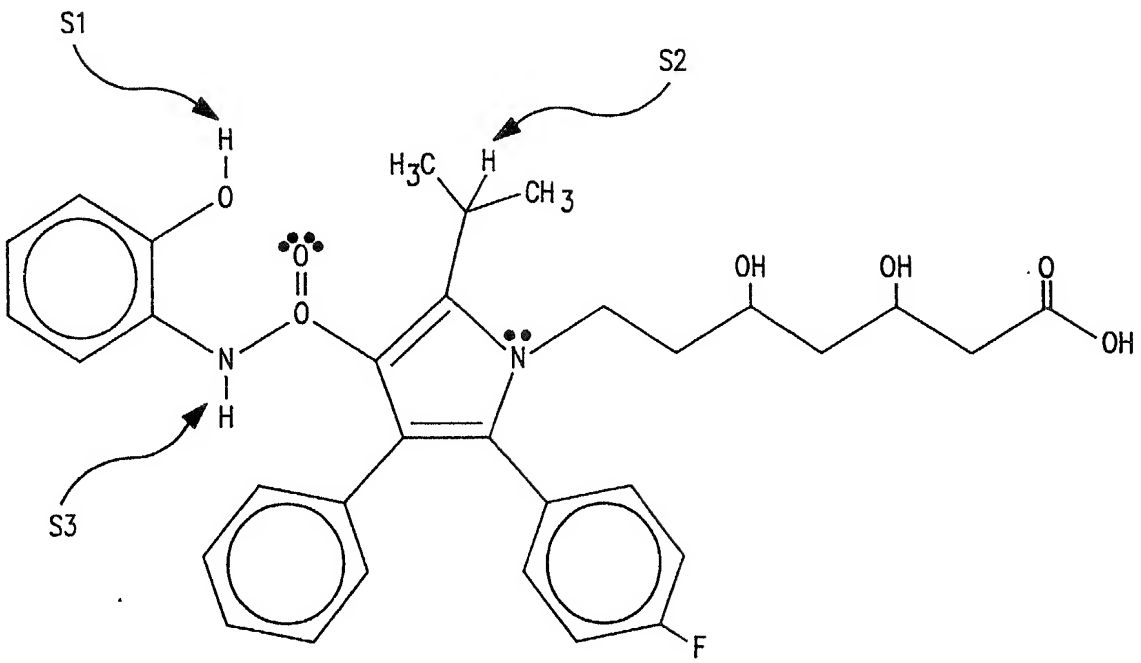

FIG. 4A

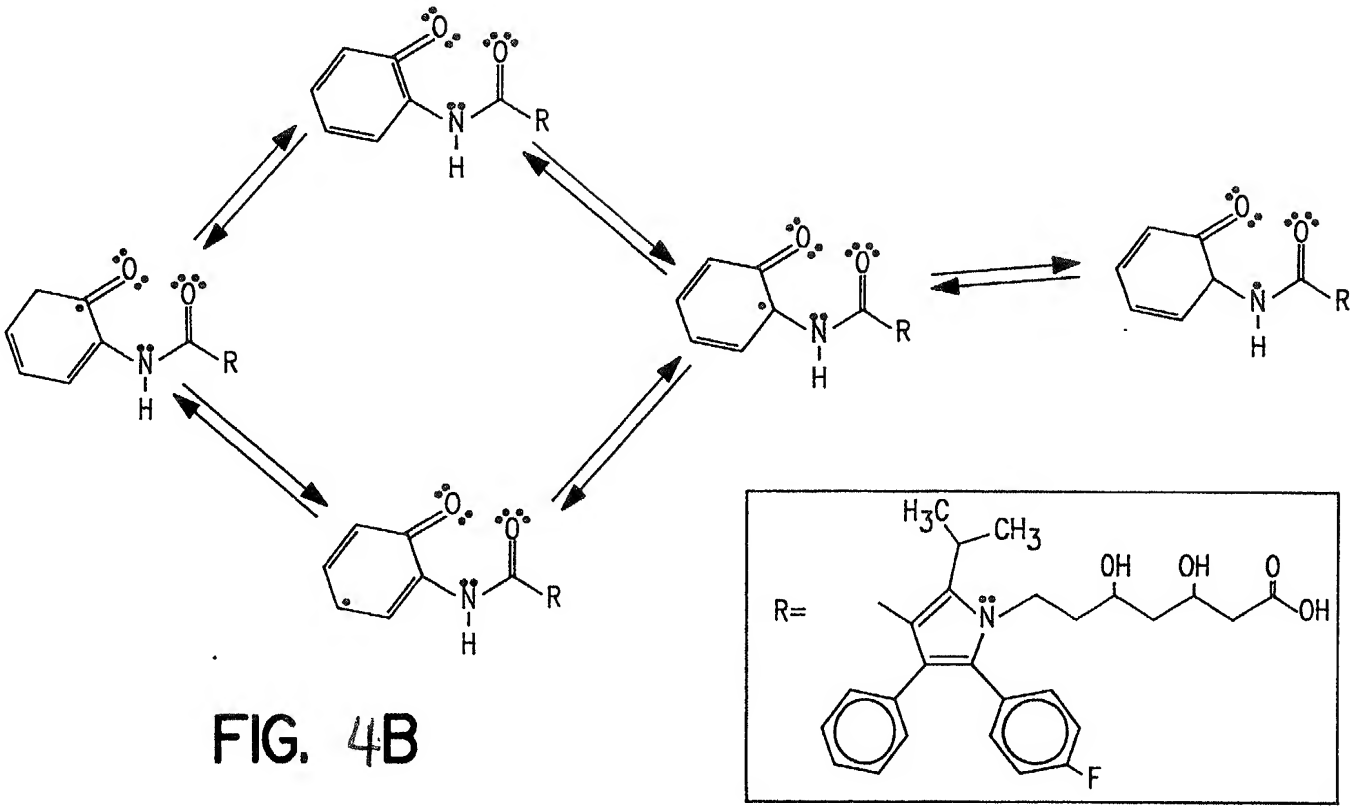

FIG. 4B

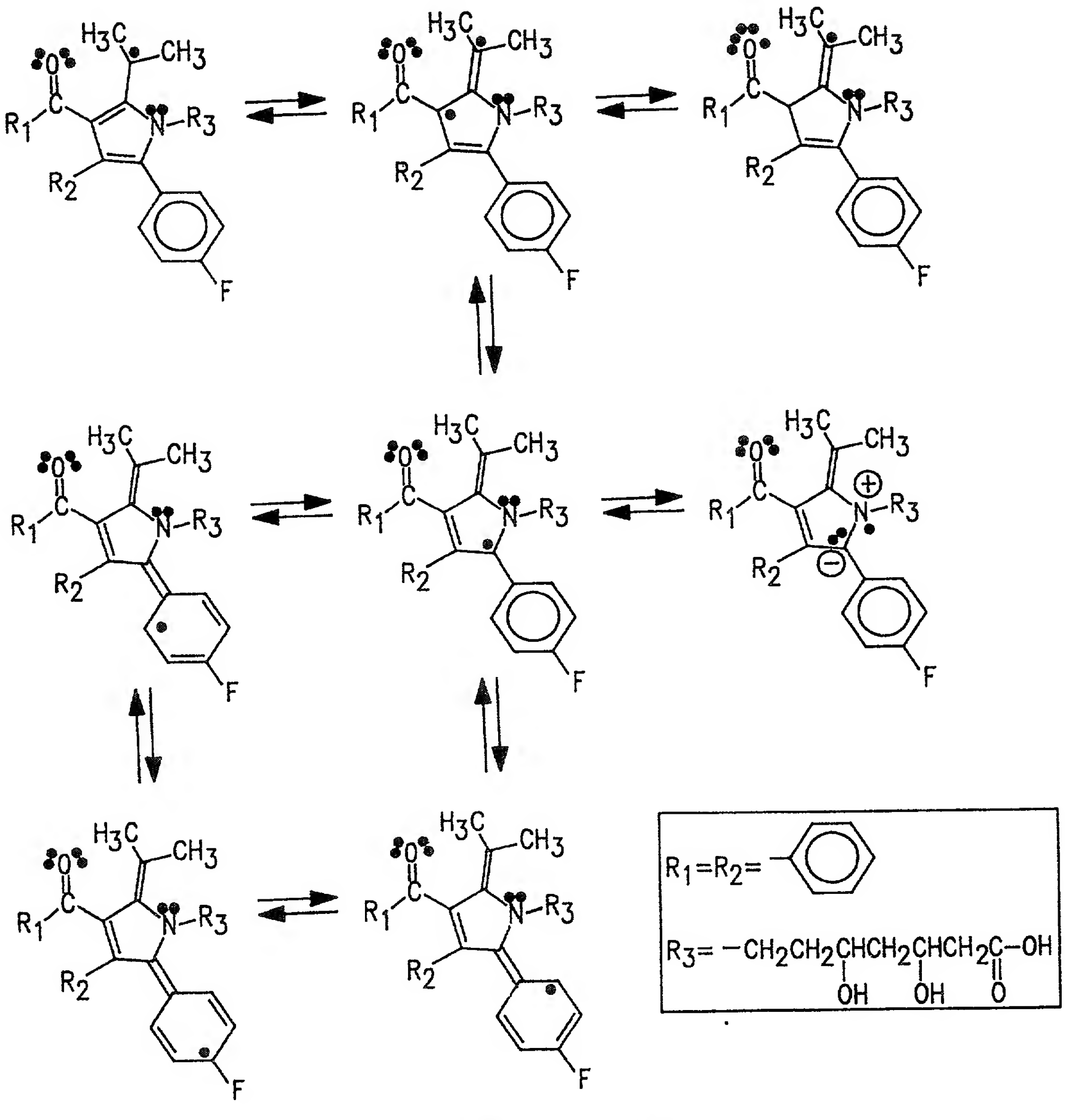

FIG. 4C

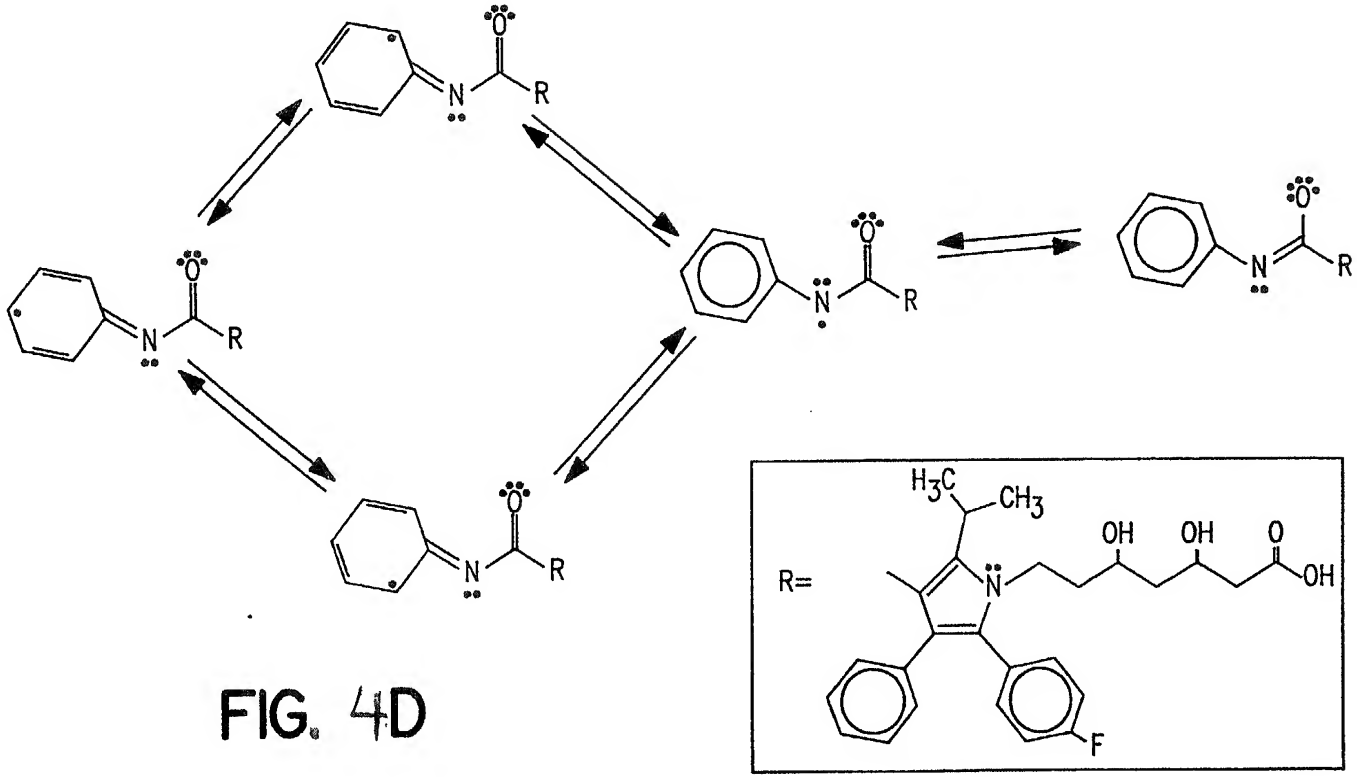

FIG. 4D

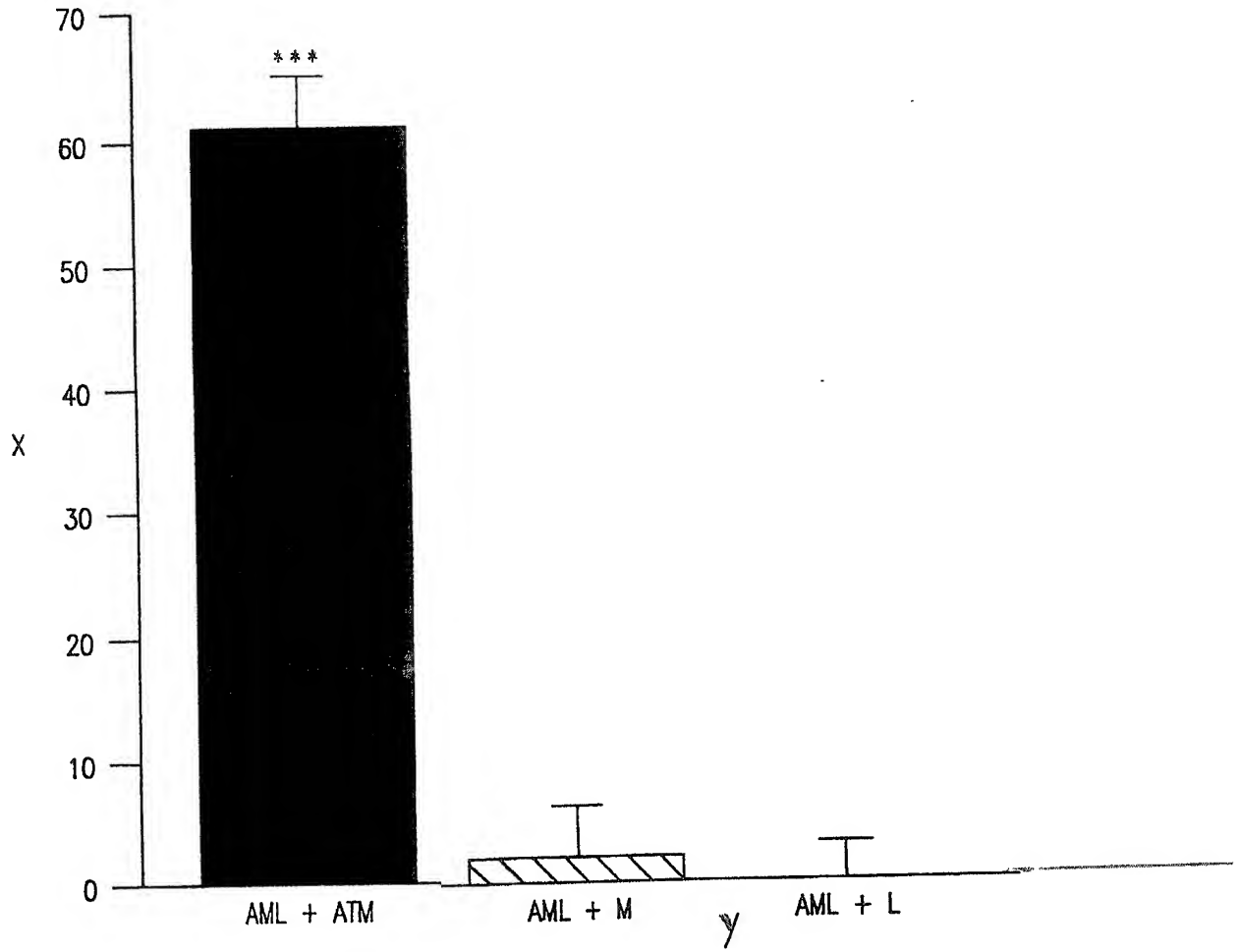

FIG. 5

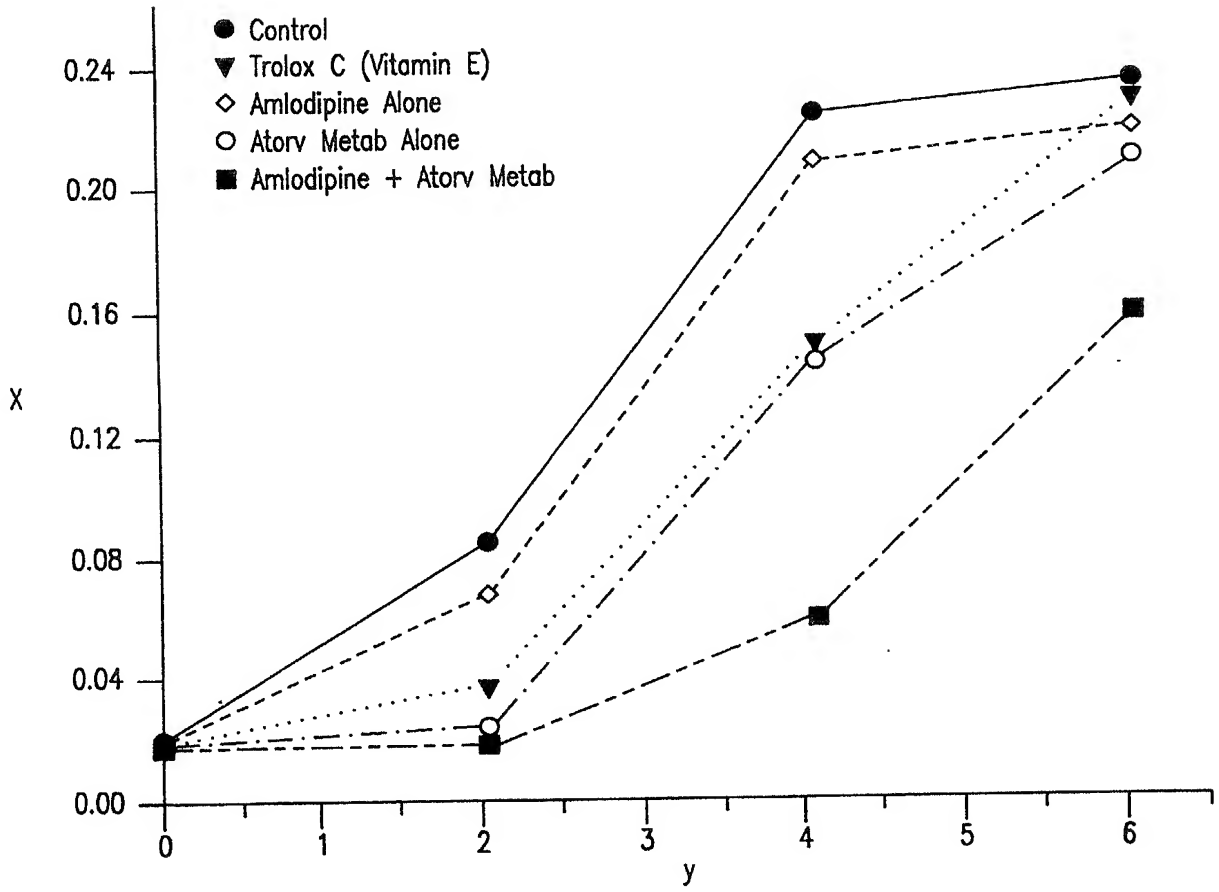

FIG. 6A

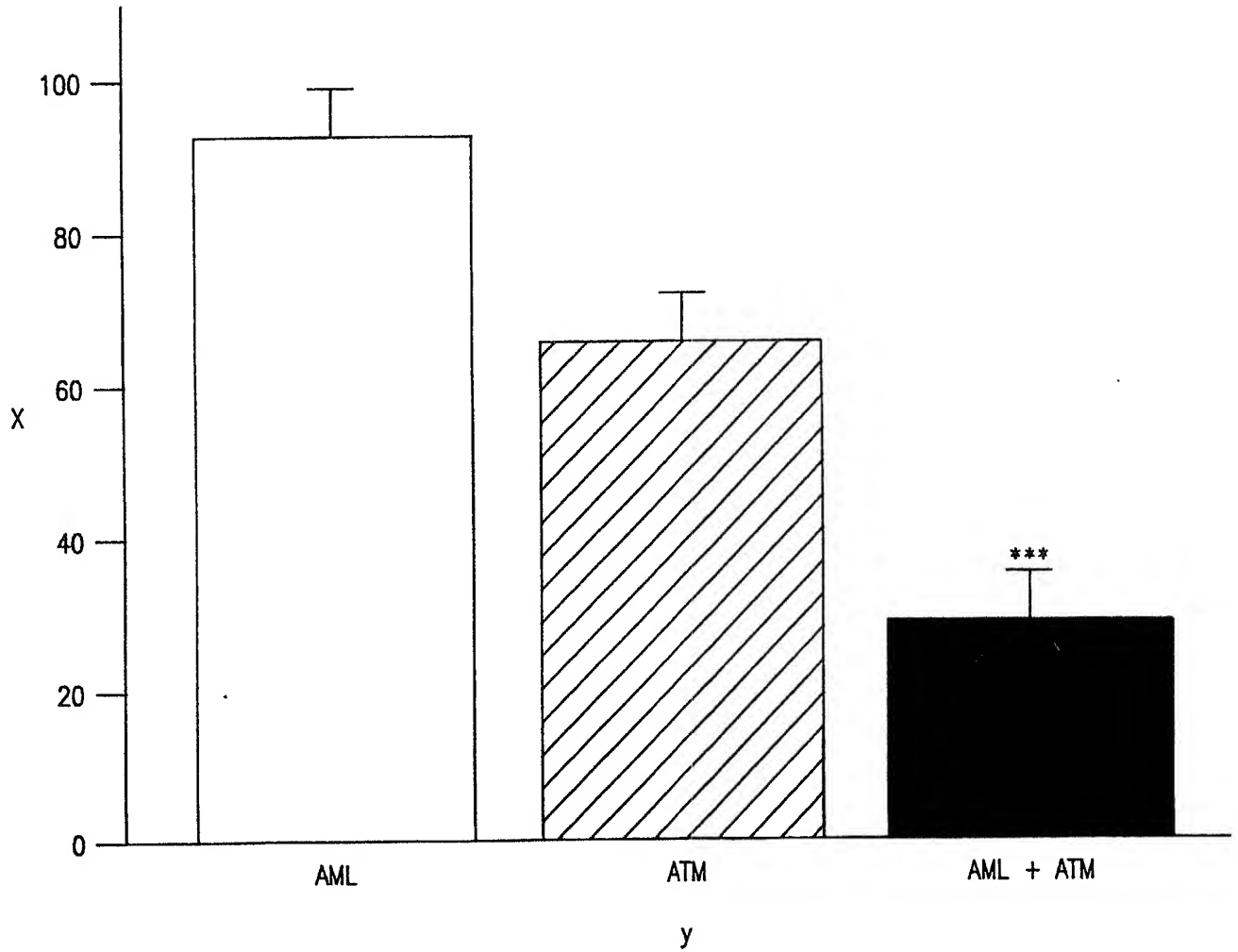

FIG. 6B

Computed Enthalpies of Formation for Atorvastatin Metabolite Radicals *

Molecule	ΔH_f (kcal/mol)
Carbon radical	−209.50
Oxygen radical	−199.89
Nitrogen radical	−192.55
Methyl radical	−193.51
Phenyl radical	−176.05
Carbon/Oxygen Diradical	−182.07
Carbon/Nitrogen Diradical	−174.25

*The smaller (i.e., more negative) the ΔH_f value, the easier to abstract the H atom from that site.

Computed Enthalpies of Formation for Amlodipine Radicals*

Molecule	ΔH_f (kcal/mol)
Carbon radical	−164.28
Nitrogen radical	−148.27

*The smaller (i.e., more negative) the ΔH_f value, the easier to abstract the H atom from that site.

FIG. 7

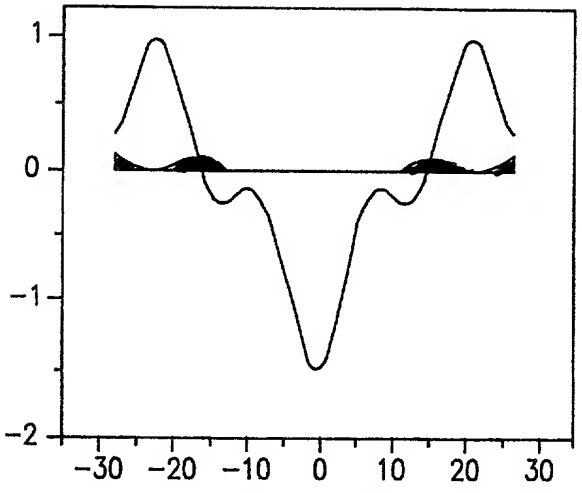

FIG. 8A

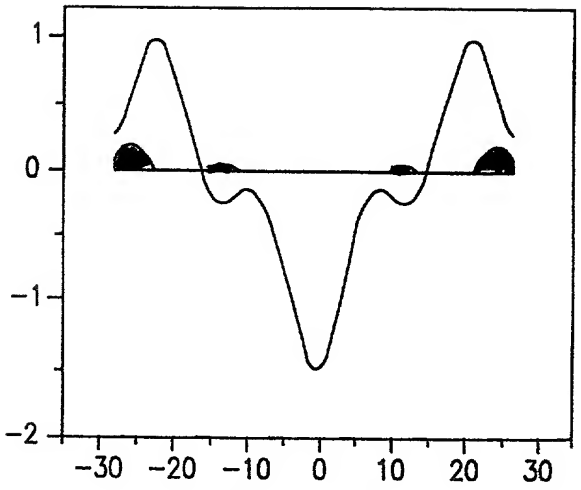

FIG. 8B

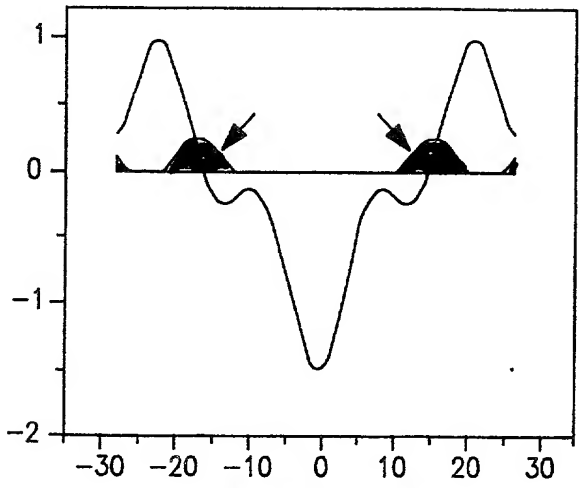

FIG. 8C

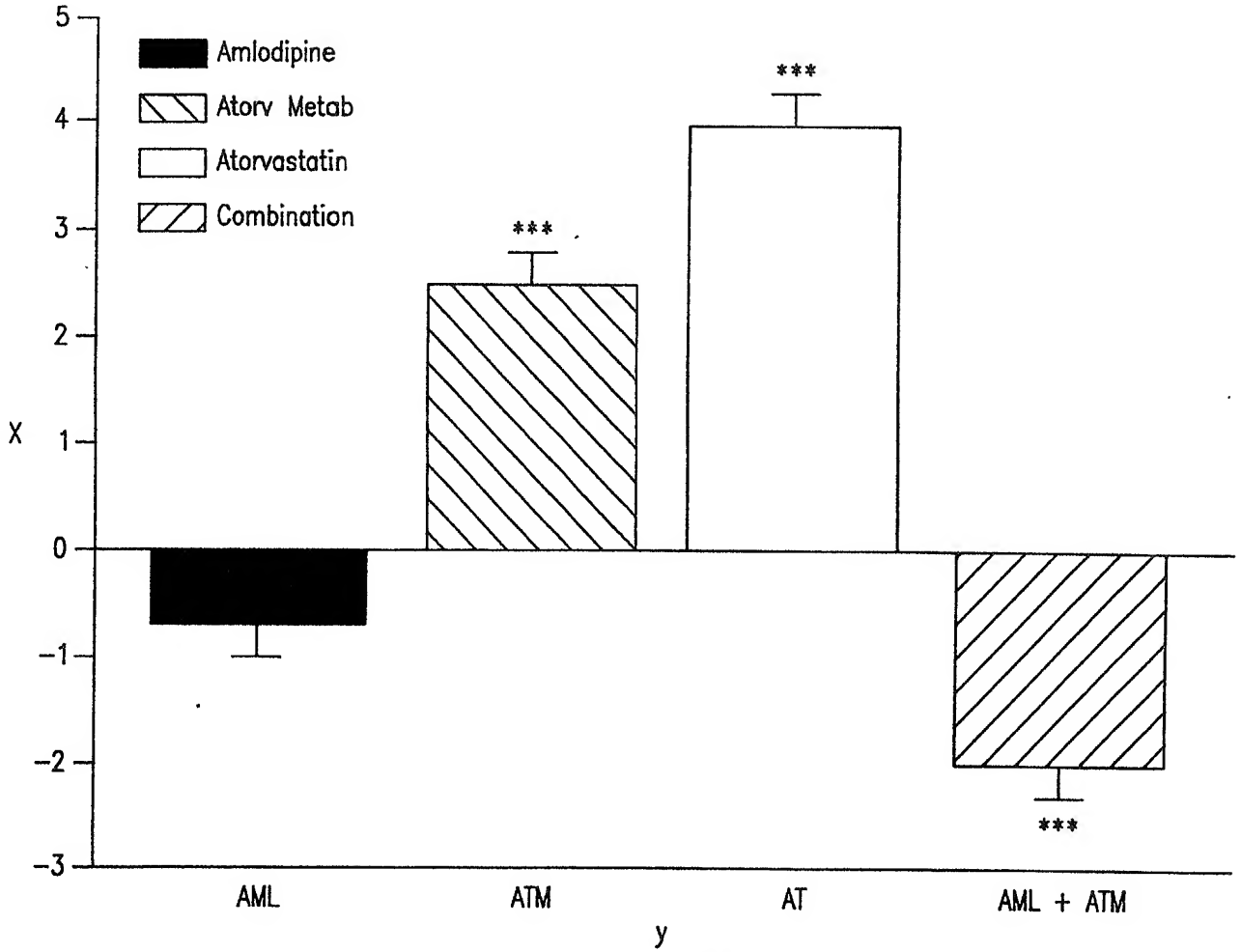
Amlodipine
Atorv Metab
Atorvastatin
Combination
5
4
3
2
1
0
−1
−2
−3
X
***
***
***
AML
ATM
AT
AML + ATM
y

FIG. 9